Ioffe Institute SEPD.04
6th Int. Symp. "Nanostructures: Physics and Technology"
St Petersburg, Russia, June 22–26, 1998.

Quantum Mott transition in mesoscopic semiconductors

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Abstract. Considering a double-barrier structure formed by a silicon quantum dot covered by natural oxide, we derive simple conditions for the conductance of the dot to become a step-like function of the number of doping atoms inside the dot, with negligible dependence on the actual position of the dopants. The found conditions are feasible in experimentally available structures.

The fabrication of Si nanostructures became possible through very recently developed new technologies [1, 2]. One unique preparation technology for individual silicon quantum dots (SQD) has been reported in [2]. They are spherical Si particles with diameters d in the range 5–12 nm covered by a 1–2 nm-thick natural SiO_2 film. Metallic current terminals made from degenerately doped Si are defined lithographically to touch each individual dot from above and from below.

To ensure metallic electrodes the donor concentration n should be $n \geq n_{\mathrm{Mott}}$, where $n_{\mathrm{Mott}} = 7.3 \times 10^{17}$ cm^{-3}. The critical concentration n_{Mott} is defined by the *Mott criterion* [3], introducing the transition to a metallic type of conductivity in a semiconductor at:

$$a_{\mathrm{B}} \times (n_{\mathrm{Mott}})^{1/3} = 0.27 \tag{1}$$

where a_{B} nm is the Bohr radius of an electron bound to a donor inside the Si crystal, in the case of phosphorus-donors $a_{\mathrm{B}} = 3$ nm [3].

As for the doping of the dot, the situation concerning a Mott transition in that small dots is much less trivial than the one described by Eq. (1). Let us consider dots with diameters $d = 10$ nm formed from n-doped Si with $n = n_{\mathrm{Mott}}$ as an illustrative example. Then each dot contains in average one donor. Note that we will consider degenerately n^+-doped electrodes with $n \gg n_{\mathrm{Mott}}$ which ensures metallic conduction up to the borders of the dot.

Real fabrication technology [2] provides a wafer with hundreds of SQDs on it with current leads towards each individual SQD. Dots in average have the same value of mean dopant concentration n, which is determined by the parent material of bulk silicon the dots are formed from. However, on the level of each individual SQD we will always have exactly *integer* number of doping atoms. If, as in the example above, the average number of dopants $\overline{N_{\mathrm{tot}}} = 1$ the actual number of donors in the dot can have values $N_{\mathrm{tot}} = 0, 1, 2, 3, \ldots$, with values larger than these very unlikely.

Our objective is to illustrate, that SQDs from the same wafer fall into several distinct sets of approximately the same conductance. The typical value of conductance for each set is nearly completely determined by the number N of donors present in a certain part of a SQD so that N labels each set of SQDs.

Summarizing the above, we need for a quantization of the conduction through a dot with N donors the following conditions:

- Size d of the dot comparable with Bohr radius: $2 < d/a_B < 5$.
- Average doping n of the dot $n \leq d^{-3}$, leading to a mean number of dopants $\overline{N_{tot}} \leq 1$, so that $N_{tot} = 0, 1, 2$ are the most probable configurations of an individual SQD.
- Doping of the electrodes $n_{el} \gg n_{Mott}$, so that current leads are perfectly metallic.
- Dot covered by an oxide layer thick enough to suppress ballistic transport through the dot.

In fact all these condition can be simultaneously satisfied for SQD fabricated with the method mentioned above [2].

1 Model system

We use a simple model of a cubic SQD with $d > 2a_B$ (we will use $d = 10$ nm for estimates), covered with an oxide layer with thickness $\delta = 2$ nm, and contacted with current terminals from below and from above. The x-axis is oriented from top to bottom along the current flow.

A tunneling current is injected into the dot via the oxide barrier from the top (source at $x = 0$) and leaves the dot at the bottom (drain at $x = d$). Due to the presence of the oxide barriers this current is non-ballistic and non-thermal. We assume that the high potential barriers associated with the oxide layers are not much affected by the voltage and the tunneling charges. We concentrate on what happens between these effective source and drain.

In the case when the dot can be regarded as an insulating system it is reasonable to assume that the applied voltage equally drops over the potential barriers and the dots. For simplicity we neglect the difference of the dielectric constants of the oxide barriers and the dot. In this approximation we can introduce an effective voltage $V_{eff} = V(d-2\delta)/d = 0.6V$ describing the part of the total transport voltage V applied between effective source and drain which drops across the dot itself.

In this rude approximation we neglect the effect of spatial quantization upon values on the ionization energy, the conductivity gap and material parameters of silicon.

2 Dot without donors

At $V_{eff} = 0$ the Fermi level inside the dot is situated in the middle of the gap, i.e. $E_g/2$ bellow the conduction band edge ($E_g = 1.14$ eV at 300 K).

As V_{eff} grows, the bottom of the (still empty) conduction band bends down accordingly. When the conduction band in the dot close to the drain aligns with the Fermi level of the emitter we expect a drastic increase in the tunneling current. This threshold V_{th} voltage for V_{eff} is given by $V_{th} = E_g/(2e)$, regardless of the number N_{tot} of dopants in the dot (as long as the dot is not yet metallic, of course). In the following we therefore limit our studies to voltages

$$|V_{eff}| \leq V_{th} = E_g/(2e) = 0.57 \text{ V}. \tag{2}$$

In this voltage range we have a d-thick barrier (formed by the dot) with always finite hight between effective source and drain. The intrinsic concentration of electrons and holes at 300 K is 1.4×10^{10} cm^{-3}. Even at this high temperature the probability to have at least one intrinsic electron in a dot with size $d = 10$ nm is only 1.4×10^{-8}. So we

would expect virtually no current in this mode. This is confirmed by direct electrical tests [2] of SQD with the required properties.

3 Single-donor channel

Let us now consider one single single donor in the dot located at x with ionization energy $E_d = 0.045$ eV (for P as a donor).

The evident channel for current flow is single-electron tunneling from the source to the empty impurity, and then from populated impurity to the drain. This channel opens as soon as V_{eff} reaches a threshold V_1 leading to a step-like increase in the total conductance of the dot. If the impurity is located near the drain, i.e. $d - a_B < x < d$ then V_1 is given by

$$V_1 = E_g/(2e) - E_d = 0.525 \text{ V}. \tag{3}$$

In contrast, for a impurity located at distances $\Delta x > 2dE_d/E_g$ (that is far) from the drain, no additional current channel via a single impurity can be opened at voltages low enough voltages defined in (2) where virtually no background current is present. In the present case this value $\Delta x = 0.8$ nm, which returns us to the above criterion: only impurities located in the immediate vicinity (defined within the accuracy a_B) of the drain contribute to the single-impurity channel.

The probability to populate an impurity from the source, and then to depopulate it towards the drain is directly related to the overlap of the atom-like impurity wave-functions with the corresponding contacts leading to a conductance G_1 of this current channel

$$G_1 \propto \exp\left(-\frac{x}{a_B}\right)\exp\left(-\frac{d-x}{a_B}\right) = \exp\left(-\frac{d}{a_B}\right). \tag{4}$$

This shows that in first approximation the conductance of this channel does not depend on x. As shown above, a single-impurity channel already only selects impurities located within a very narrow range of x close to the drain, Eq. (4) gives an additional argument for the independence of this channel conductance G_1 on the actual location of the impurity inside this thin layer near the drain.

4 Two-, three-, multi-donor channel

The above consideration shows, that due to the bend of the bottom of conduction band following the transport voltage, there is no chance to notice current flowing through a sequential chain of impurities, connecting source and drain. The contribution of such a chain will be totally masked by the current flowing directly via the conduction band. The only way for multiple impurities to manifest themselves in quantized conductance is to form multiple *parallel* singe-impurity channels situated close enough to the drain as considered above.

Therefore, if $N > 1$ impurities fall into the thin layer near the drain, we will see a switching-on of an N-fold channel with conductance

$$G_N = NG_1 \tag{5}$$

at the same threshold voltage $V_{\text{eff}} = V_1 = 0.525$ V as for a single-donor channels.

Discussion

All the above considerations are only valid as long as the dot itself can be regarded as an insulating system. As the number of donors in a SQD grows, the dot becomes a metallic particle, and the conduction band edge in the dot aligns with the Fermi level of the electrodes. In a very simple estimate we define this transition to a metal when the total volume of N donors with an individual volume of $4\pi/3 \times a_B^3$ exceeds the volume of the dot. This is an exaggerated version of the Mott criterion (1) which holds not only in bulk, but in a small structure, too. For the analyzed example from above this gives $N_{tot} = 8$ as a limiting value. The practically interesting set $0, 1, 2, 3, \ldots$ for both N_{tot} and N considered above is still far bellow this limit.

Quite a number of other mechanisms of electron transport might take place in this system, the main one being resonant tunneling. Surprisingly, even taking into account such other mechanisms [4] does not change much the main idea of the present paper.

Acknowledgments

Useful discussions with M. Kupriyanov and S. Oda are gratefully acknowledged. This work was supported in part by the Russian Foundation for Basic Research and by the Russian Program for Future Nanonelectronic Devices.

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